

Toluene  
108-88-3 | DTXSID7021360

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

## Model Results

**Predicted value:** 24.6

**Global applicability domain:** Inside

**Local applicability domain index:** 6.42e-01

**Confidence level:** 7.94e-01

## Nearest Neighbors from the Training Set

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1,2-Dibromoethane

**Measured:** 15.1

**Predicted:** 13.4

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Isoprene

**Measured:** 20.0

**Predicted:** 15.6

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Thiophene, 3-methyl-

**Measured:** 5.25

**Predicted:** 7.49

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4-Vinylcyclohexene

**Measured:** 166

**Predicted:** 158

Image not found

5-Ethylidene-2-norbornene

**Measured:** 110

**Predicted:** 134